

[Buddha Series]

Course - B.Tech

Subject - Engg. Chemistry (BAS102/BAS-202)

Unit - I

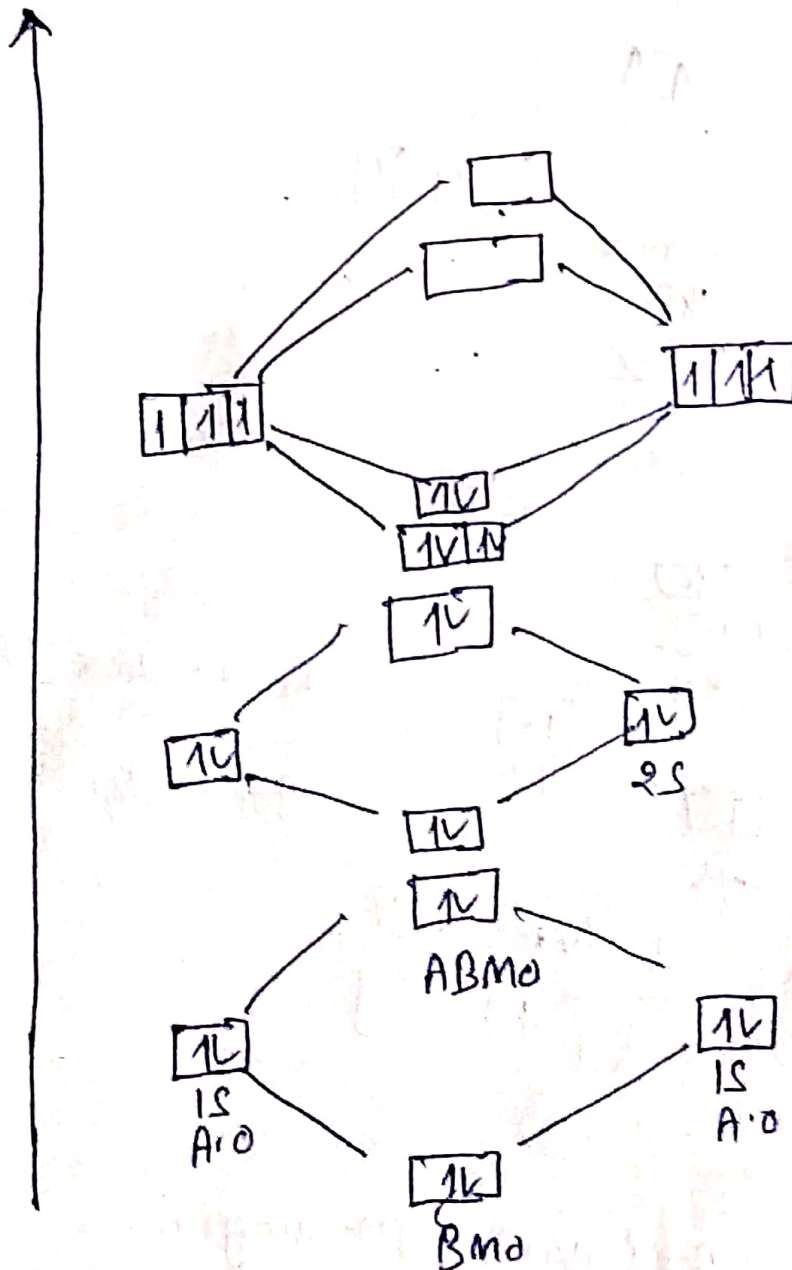
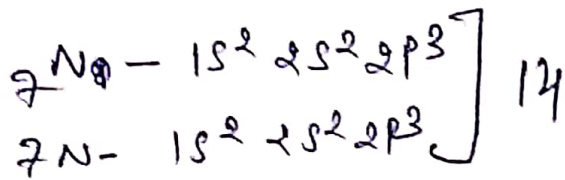
Topic - Atomic and Molecular Structure

By

Dr. Rajesh Kumar Mall

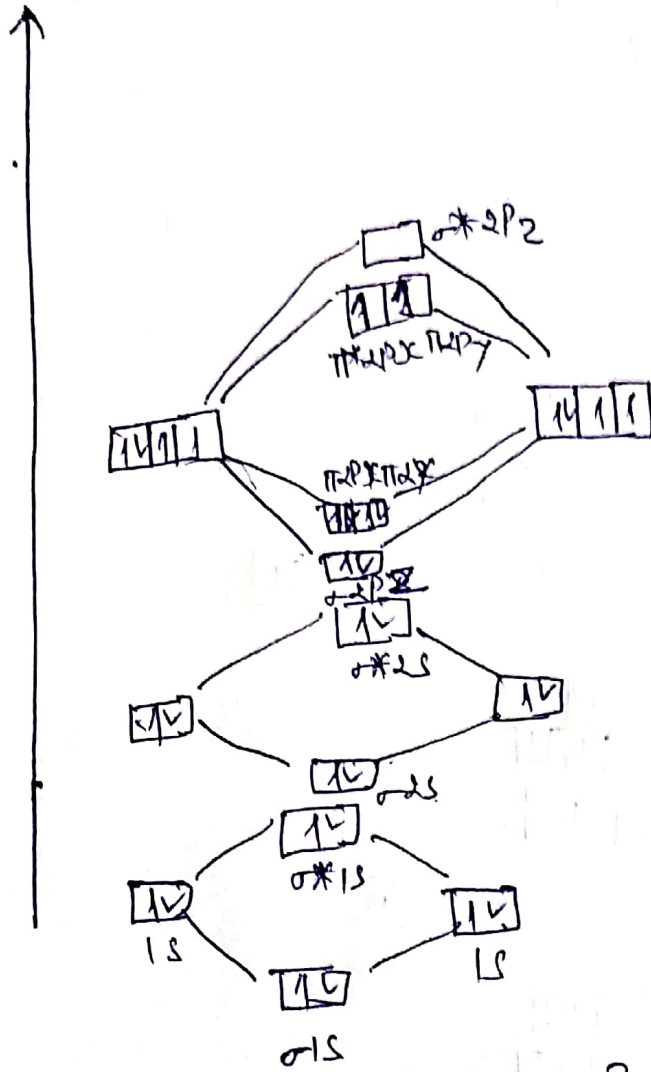
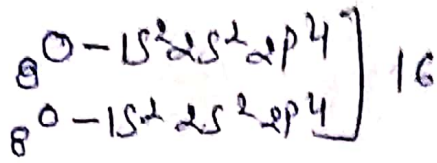
① Draw the molecular orbital diagram of N_2 molecule
 Give its bond order and magnetic behaviour.

Molecular orbital diagram of N_2 molecule.



② Draw the m.o diagram of O_2 molecule and its magnetic behaviour (2009, 2013, 2019).

Molecular orbital diagram of O_2 molecule.



Bond order \propto $\frac{\text{Bond order}}{\text{Bond length}}$

$$\begin{aligned}
 \text{Bond order} &= \frac{1}{2} [N_b - N_a] \\
 &= \frac{1}{2} [10 - 6] \\
 &= 2
 \end{aligned}$$

magnetic Behaviour - paramagnetic

Bond order of $N_2 = 3$	$F_2 = 1$	$NO = 2.5$
$O_2 = 2$	$CO = 3$	$NO^+ = 3$

Q) What are liquid crystals, Give its classification and application also (2024)

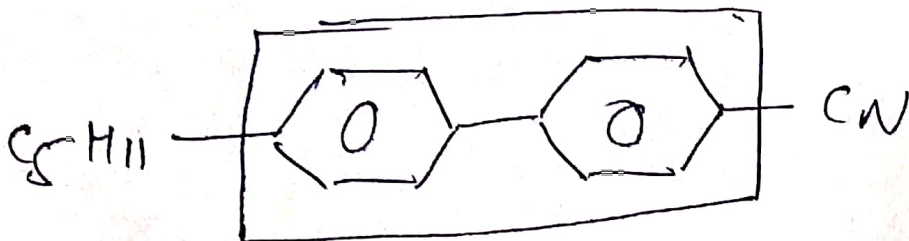
[Liquid crystalline state] ①

Liquid crystals are substances that exhibit a phase of matter that have properties b/w liquid and those of solid crystal. (Hery 4'4'4')

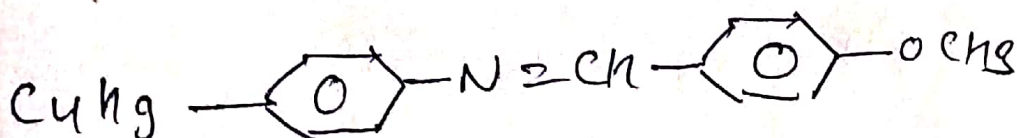
These phase have translucent or cloudy appearance. Liquid crystalline phase are also called mesomorphic phases.

Essential requirement for the L.C.

- ① Presence of carboxyl group at end.
- ② molecule of anisotropic in nature.
- ③ Absence of bulky functional group.
- ④ presence of unsaturation
- ⑤ molecule have some rigidity in center and ends must be flexible



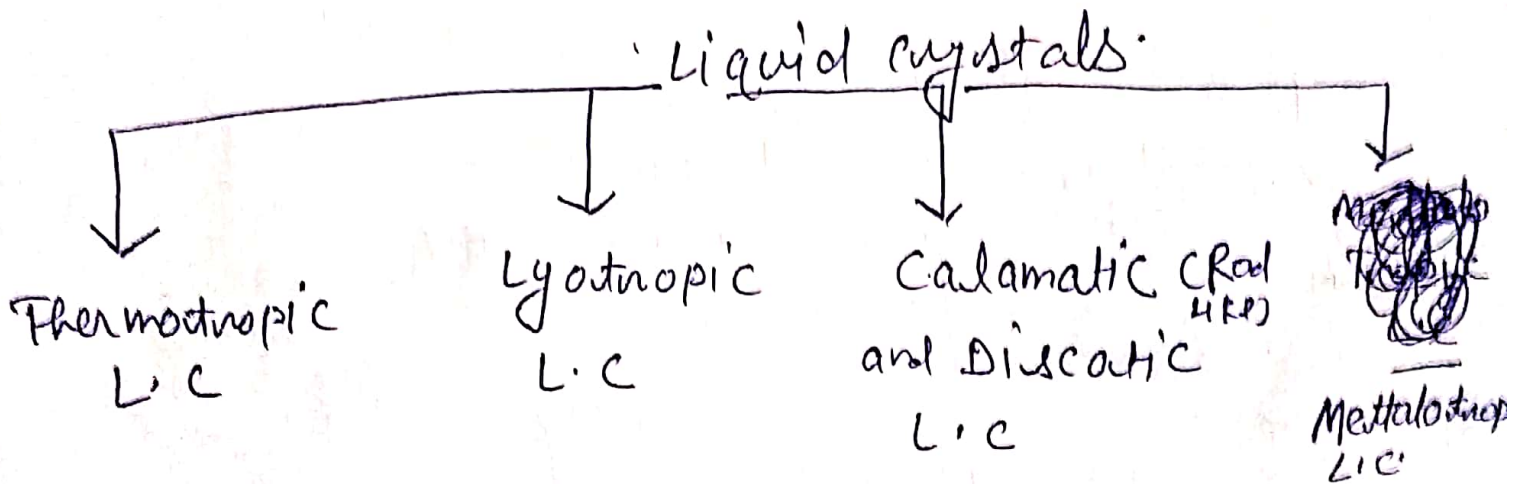
Rigid Rod like part (Mesogen) -



molecules which form liquid crystals.

- ① cholesteral ester
- ② phenyl benzoates
- ③ paraffins.
- ④ Glyco lipids
- ⑤ cellulose derivative.

classification of liquid crystal.



Application of Liquid crystal.

- ① Liquid crystal display (LCD). A LCD is a thin flat display device made up of many number of colours or monochrome in front of light source or reflector. LCD used in notebook, small computer, Light emitting diode (LED). It is much thinner than cathode Ray tube (CRT).
- ② Liquid crystal thermography = chiral nematic or cholesteric L.C used for detecting tumors cancer in human body by the method called thermography.
- ③ Gas liquid chromatography \Rightarrow L.C have property of crystalline solid and liquids so they are used in gas liquid chromatography.
- ④ L.C are used as solvent for the study of anisotropic molecules by the method spectroscopically.
- ⑤ L.C are used in making digital thermometer.

Q) Describe the structure and application of Graphite and Fullerenes. Explain the reason for electrical and Lubrication properties of Graphite (2023).

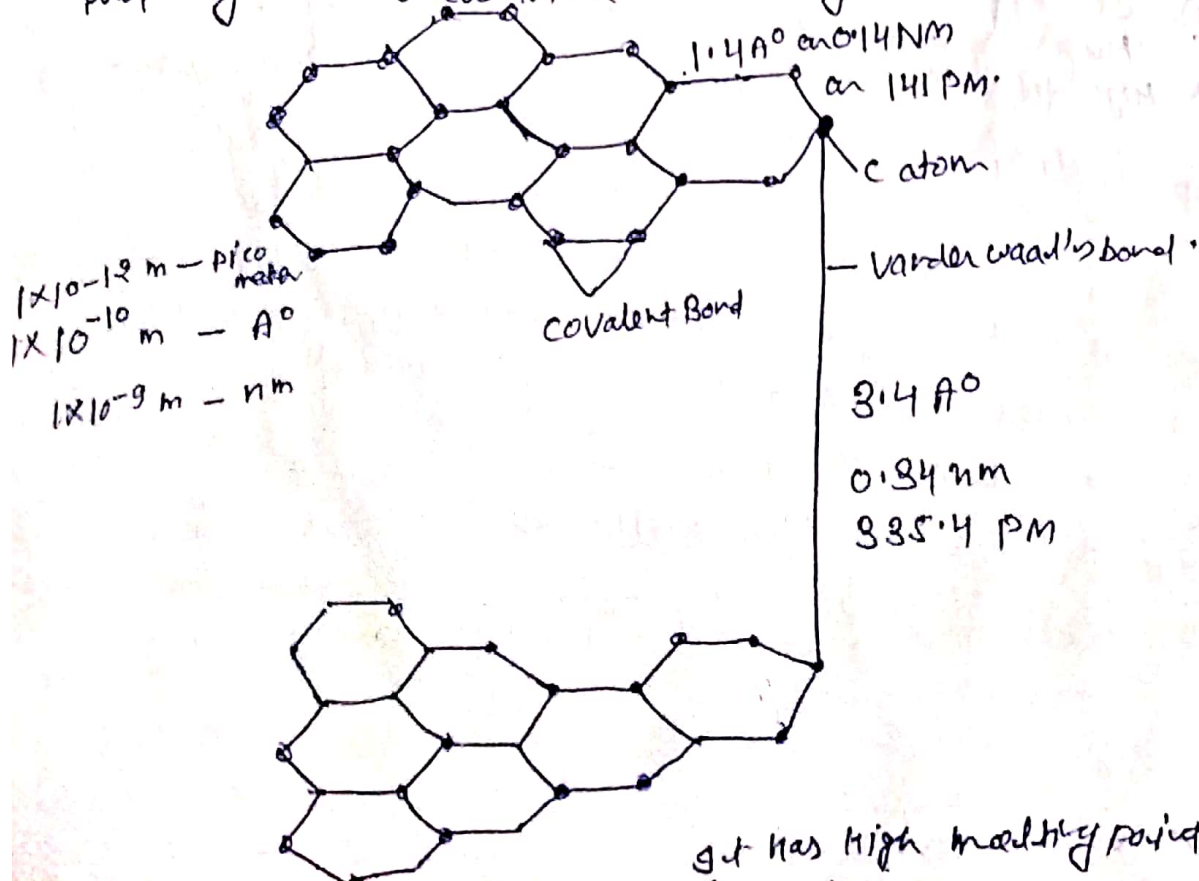
[Graphite]

Amorphous - coal
 Cryst - Diamond, Graphite, Fullerene

Graphite is Allotrop of carbon. In graphite atoms are arranged in layers. It is of two type α and β Graphite. It has sandwich like structure.

In graphite carbon atom is arranged in hexagon and hexagon form a plane. Each carbon atom in hexagon attached to only three carbon atom by covalent bond. The fourth e- is participating in a weak Vander waal's type of bonds between the layers. Graphite show sp^2 hybridisation.

Due to presence of weak Vander waal's bond cleavage is facile which give excellent Lubricative property and also electrical conductivity to Graphite.



Type of Graphite.

① α - Graphite - Hexagonal arrangement

ABAB Type arrangement

② β Type Graphite, it has Rhombohedral Arrangement.

ABCABC Type Arrangement

Properties of Graphite.

- ① It is gray colour crystalline solid
- ② It is soft and soapy in touch.
- ③ Good conductor of electricity.
- ④ It behaves like solid lubricant.
- ⑤ High strength and good chemical stability.
- ⑥ High thermal conductivity low coefficient of thermal expansion.

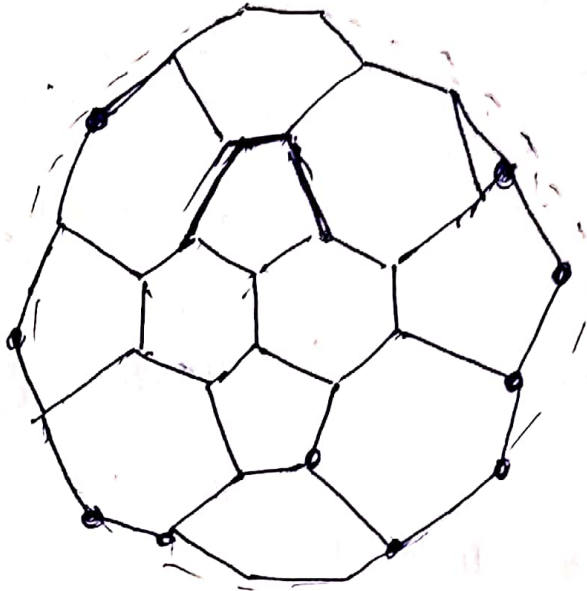
Application - It is used in pencil lead.

- ① It is used in making moderator Rod.
- ② As heating element for electric furnaces.
- ③ Electrode for welding
- ④ casting moulds for metal alloys and ceramics.
- ⑤ Rocket Nozzles.
- ⑥ Electrodes in batteries.
- ⑦ In purification devices.

[Fullerenes]

①

Fullerenes is an allotrop of carbon. It was discovered by H. Kroto and Richard Smalley and named after Richard Buckminster Fuller.



C₆₀
C₇₀
C₈₀
C₉₀
C₁₄₀

Fullerene C₆₀

football

Structure - It is hollow spherical soccer ball like structure, so it is also called Bucky ball.

- ② The structure of fullerenes each Carbon atom is sp² hybridized and arranged in hexagon and pentagon.
- ③ It is represented by C₆₀
- ④ In one molecule of C₆₀ there are 20 Hexagon and 12 pentagon.
- ⑤ They are arranged in such a way that two pentagon never share their wall.

[Application of fullerenes]

2

- ① As super conductor - It can be used as super conductor when doped with alkali metals.
- ② Carbon nanotube (CNT) - It is used in making carbon nanotubes. Carbon fiber made from organic polymer are used to strengthen light weight high-tech material such as carbon/epoxy resin used in golf clubs, tennis racquet.
- ③ It is used ^{antibodies} detection of cancer cell Tumor cells in brain and heart.
- ④ It is used in oral nano medicines.
- ⑤ used as catalyst and used as smart materials.

Q) What are nano materials. Give their application in different field and preparation also (2024).

[Nanomaterials]

①

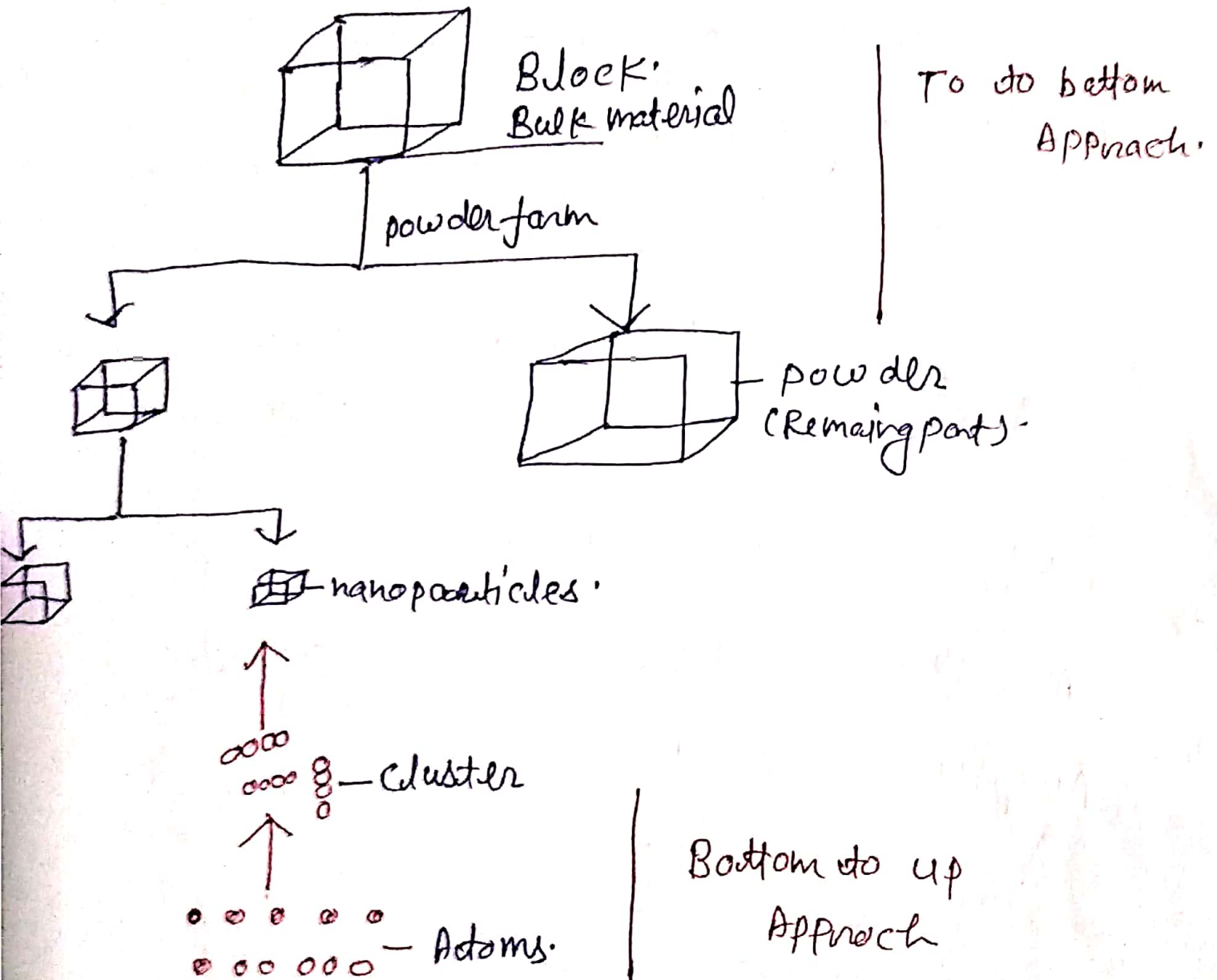
The term nano originated from Greek word nanos means dwarf. The material which have particle size in between $1-100 \text{ nm}$.

Nanotechnology \Rightarrow The manipulation of matter on atomic & molecular scale.

Si	Simple properties insulator	prop. of nanomaterial conductor / semi conductor
Pt	poison material	catalyst
Al	stable	combustible
Au (gold)	melts 1065°C	300°C .

Preparation of nanomaterials.

- ① Top down Approach
- ② Bottom to up approach.



Application of Nanomaterials/Nanotechnology.

① In medical field. Some nanoparticles are developed that they deliver drug to specific type of cell which allow to direct treatment of those cells.

② Electronics - Due to nanotechnology reduce the size of transistors in integrated circuits.
~~Iron ore~~

③ Environment ⇒

① Iron nanoparticle cleaning organic solvents that are polluting ground H₂O

② Ag nanoparticle reduce the production of byproduct in manufacturing propylene oxide.

③ Silicon nanowires embedded in polymer result low cost but high efficiency solar cells.

④ Consumer product - 1) Ag nanoparticle is used in making odour resistant clothes.

⑤ Spontis - Increasing strength of Tennis racket by adding nanotubes.

Nanoparticle is used in manufacturing golf club shaft.

Q) What is Green chemistry. Give its 12 principle of Green chemistry. (2024)

[Green chemistry]

The practice of chemistry in a manner that maximise its benefits while eliminating or at least greatly reducing its adverse impact has come to be known as green chemistry.

The 12 principles of green chemistry as given by Anastas and Clark.

12 principles of green chemistry.

- 1) prevention
- 2) Atom economy
- 3) Less Hazardous chemical synthesis.
- 4) Designing safer chemicals.
- 5) Safe solvent
- 6) Design for energy efficiency.
- 7) use of Renewable Feedstocks.
- 8) Reduce Derivatives.
- 9) catalysis.
- 10) Design for degradation
- 11) Real time analysis for pollution prevention
- 12) Safer chemistry for accident prevention.

⑦ Give the conventional and green method for the synthesis of paracetamol.

[Paracetamol]

⑧

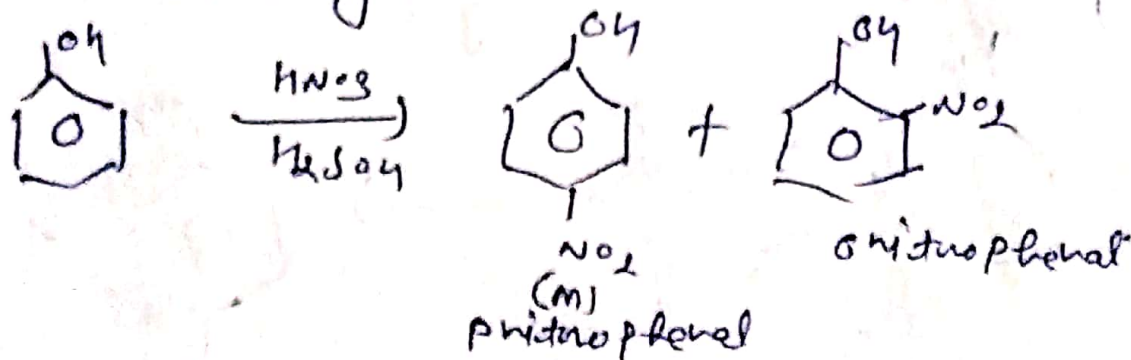
Paracetamol is used to treat fever and reduce mild pain. It is an antipyretic drug.



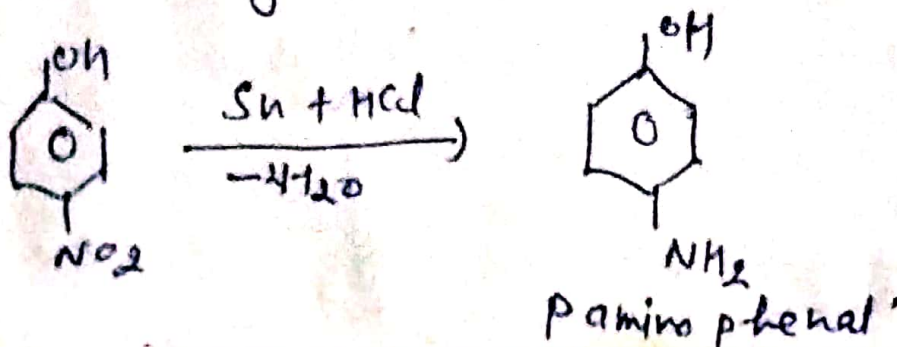
N-(4-hydroxyphenyl)ethanamide.

conventional method - It is synthesized from phenol in three steps.

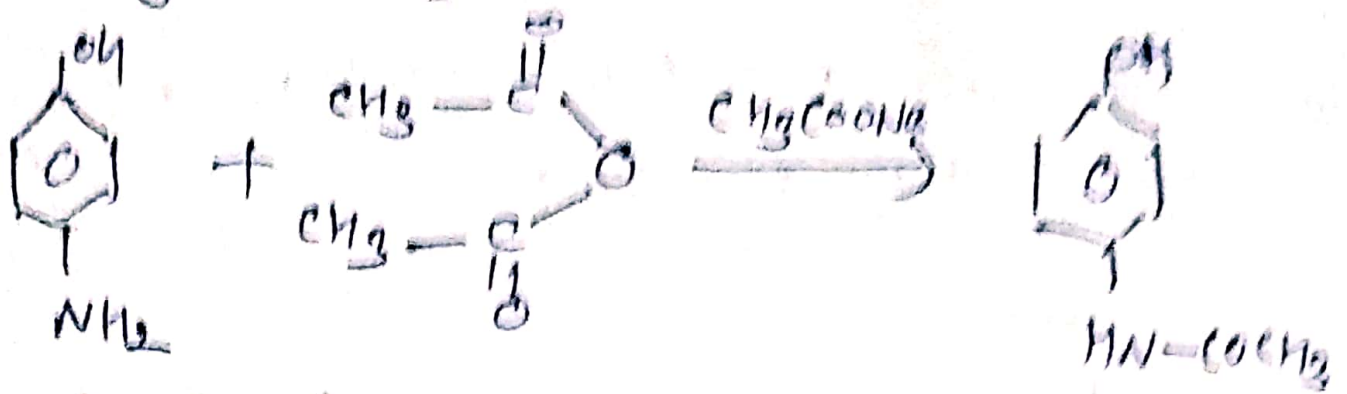
① Nitration of phenol.



② Reduction of p-nitrophenol.



③ Acetylation of p amino phenol



p amino phenol

Acetaminophen
(paracetamol)

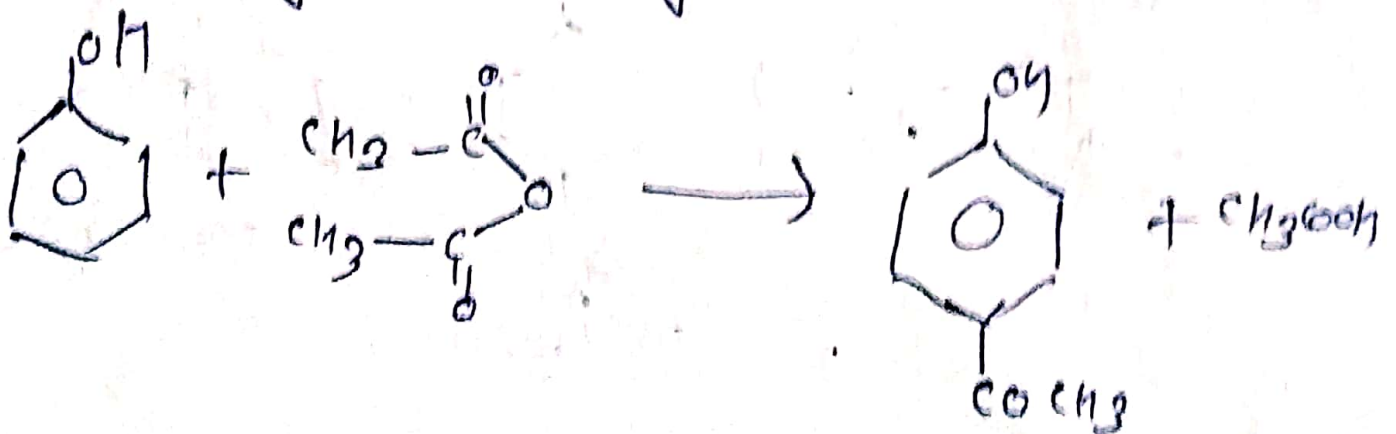
① Acid anhydride

② Sn is used

Green method

In this method starting material is phenol and it also required 3 step

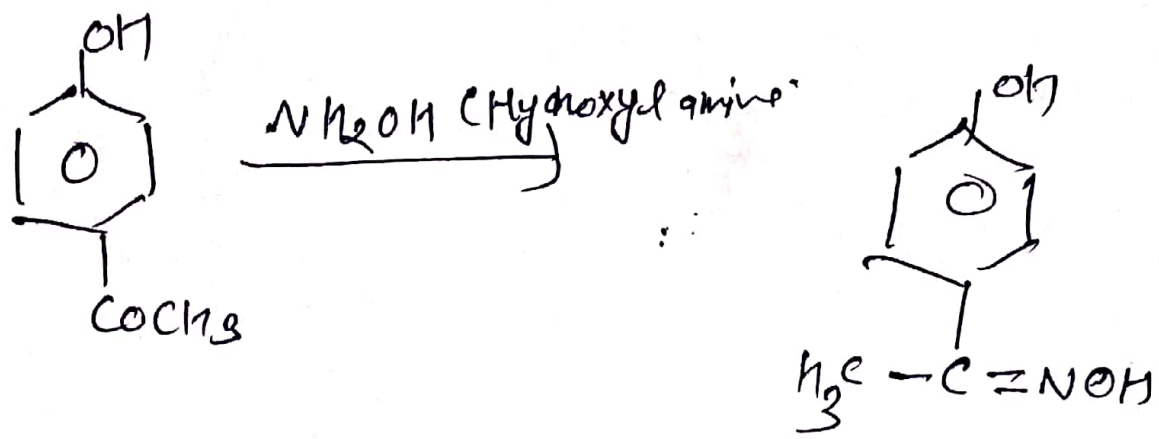
④ Acetylation of phenol



p acetophenol

(4 hydroxy phenone)

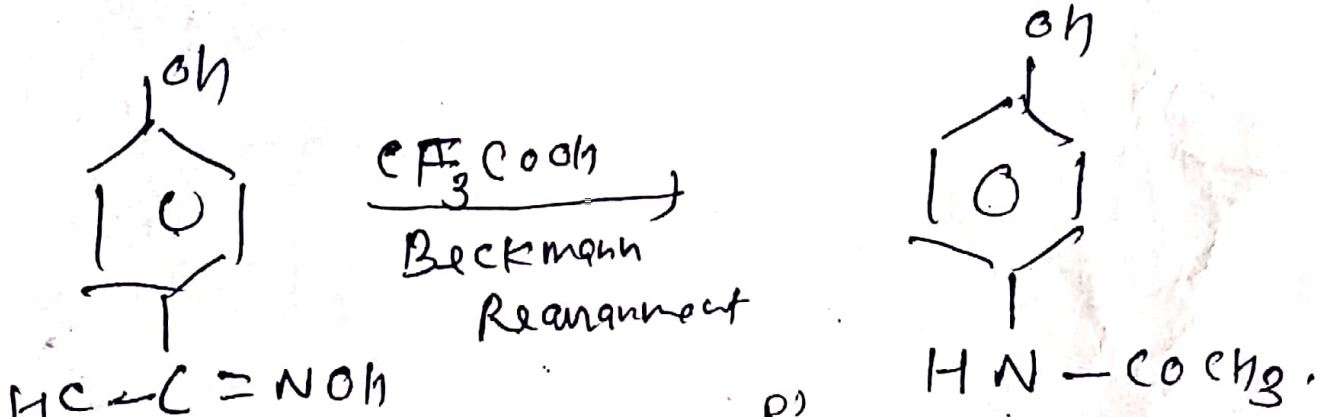
② stop - Reach p acetophenol with hydroxyl amine to form ketoxime



(Oxime - class of nitrogen containing organic compound)

Ketoxime

③ Oximes undergo Beckmann rearrangement to produce paracetamol



$$\begin{array}{c}
 R' \\
 \diagdown \\
 C = N - OH \\
 \diagup \\
 R
 \end{array}
 \longrightarrow
 \begin{array}{c}
 R' \\
 \diagdown \\
 C = O \\
 \diagup \\
 NH \\
 \diagdown \\
 R
 \end{array}$$

Beckmann - Oxime to amide, in acidic conditions

Amide - Have carbonyl functional group which is linked to amine and hydrocarbon